



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:12 PM UTC

PDB ID : 2HTM / pdb_00002htm
Title : Crystal structure of TTHA0676 from *Thermus thermophilus* HB8
Authors : Sugahara, M.; Kunishima, N.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2006-07-26
Resolution : 2.30 Å (reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

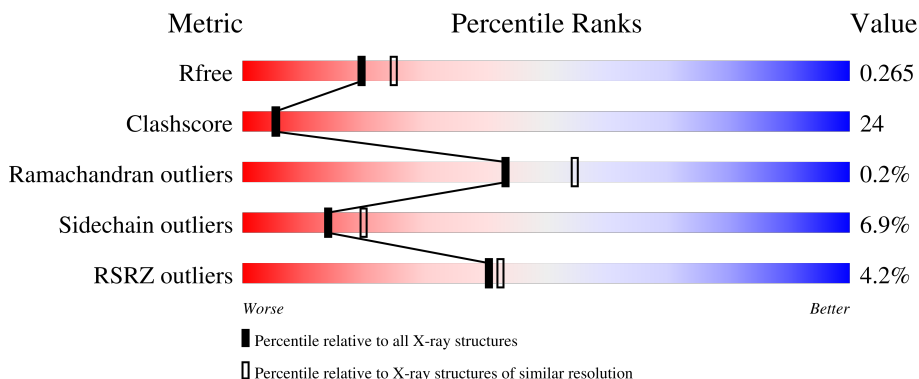
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



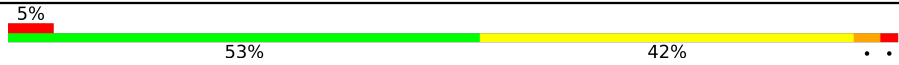


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	268	 3% 44% 35% 8% 13%
1	B	268	 4% 47% 32% 7% 13%
1	C	268	 3% 47% 37% 6% 10%
1	D	268	 4% 46% 36% 5% 13%
2	E	64	 3% 62% 33% 2% 2%

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Mol	Chain	Length	Quality of chain
2	F	64	
2	G	64	
2	H	64	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 9392 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Thiazole biosynthesis protein thiG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	234	Total 1759	C 1127	N 305	O 320	S 7	0	0	0
1	B	233	Total 1750	C 1122	N 304	O 317	S 7	0	0	0
1	C	241	Total 1809	C 1160	N 315	O 327	S 7	0	0	0
1	D	234	Total 1759	C 1127	N 305	O 320	S 7	0	0	0

- Molecule 2 is a protein called Putative thiamine biosynthesis protein ThiS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	Se			
2	E	64	Total 489	C 311	N 80	O 95	Se 3	0	0	0
2	F	64	Total 489	C 311	N 80	O 95	Se 3	0	0	0
2	G	64	Total 489	C 311	N 80	O 95	Se 3	0	0	0
2	H	64	Total 489	C 311	N 80	O 95	Se 3	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	1	MSE	MET	modified residue	UNP Q5SKG8
E	23	MSE	MET	modified residue	UNP Q5SKG8
E	61	MSE	MET	modified residue	UNP Q5SKG8
F	1	MSE	MET	modified residue	UNP Q5SKG8
F	23	MSE	MET	modified residue	UNP Q5SKG8
F	61	MSE	MET	modified residue	UNP Q5SKG8
G	1	MSE	MET	modified residue	UNP Q5SKG8
G	23	MSE	MET	modified residue	UNP Q5SKG8

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Chain	Residue	Modelled	Actual	Comment	Reference
G	61	MSE	MET	modified residue	UNP Q5SKG8
H	1	MSE	MET	modified residue	UNP Q5SKG8
H	23	MSE	MET	modified residue	UNP Q5SKG8
H	61	MSE	MET	modified residue	UNP Q5SKG8

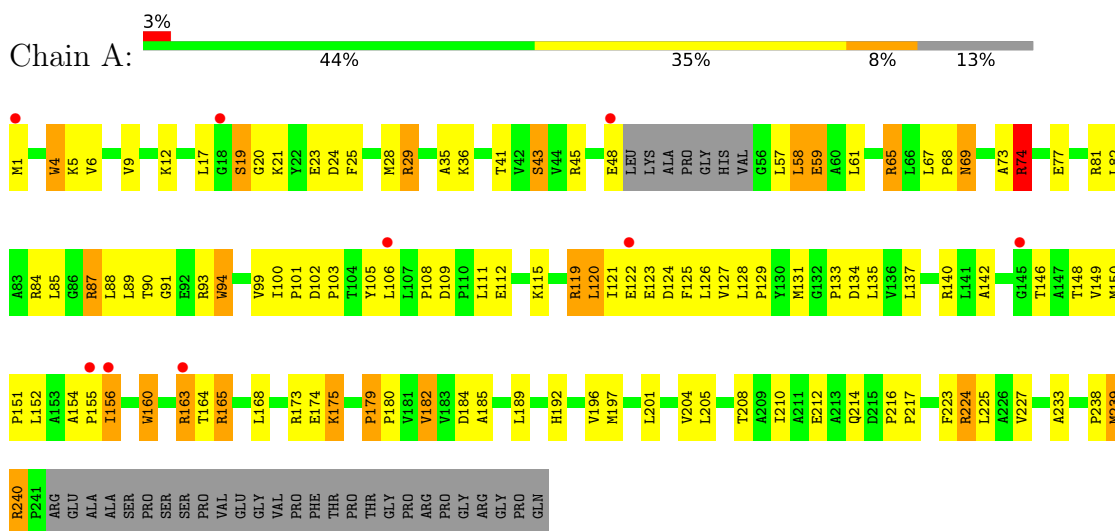
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	89	Total O 89 89	0	0
3	B	60	Total O 60 60	0	0
3	C	94	Total O 94 94	0	0
3	D	58	Total O 58 58	0	0
3	E	10	Total O 10 10	0	0
3	F	14	Total O 14 14	0	0
3	G	30	Total O 30 30	0	0
3	H	4	Total O 4 4	0	0

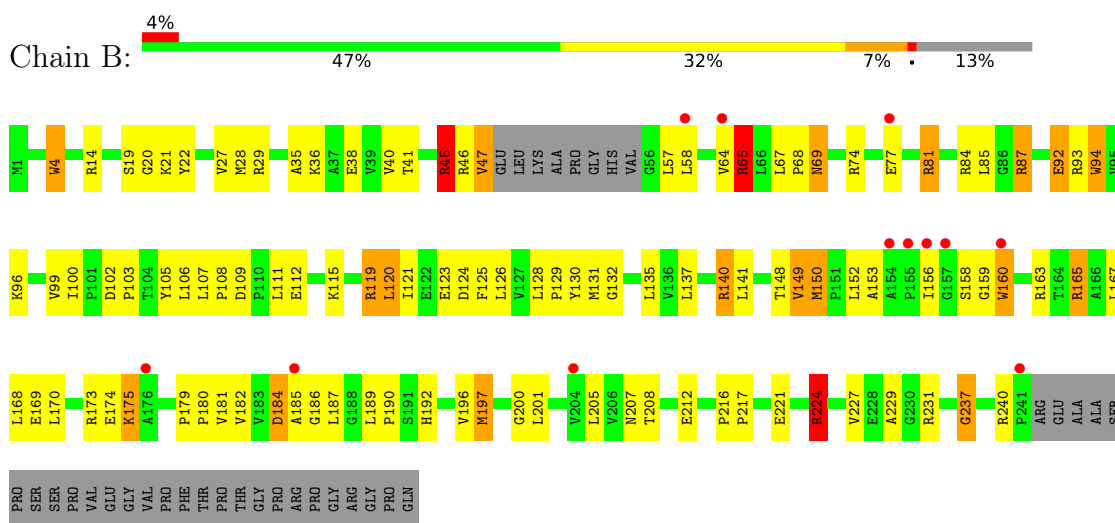
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Thiazole biosynthesis protein thiG

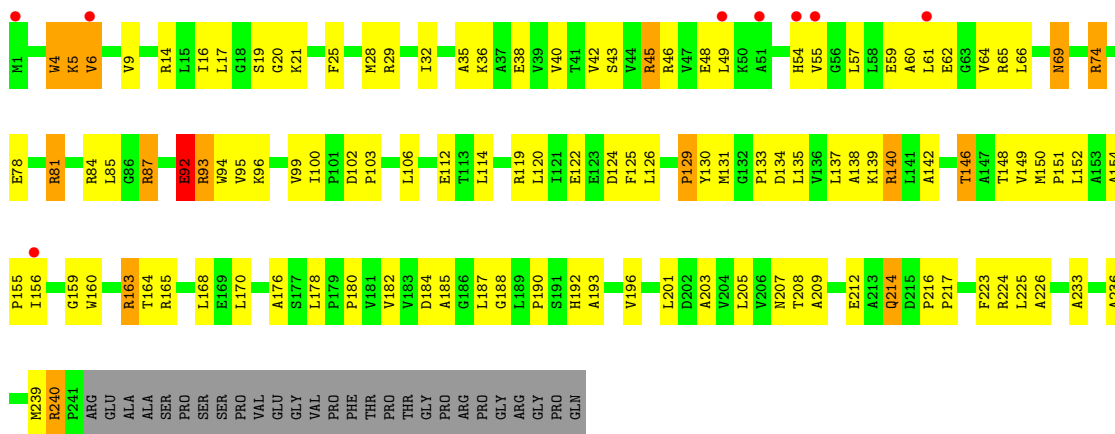


- Molecule 1: Thiazole biosynthesis protein thiG

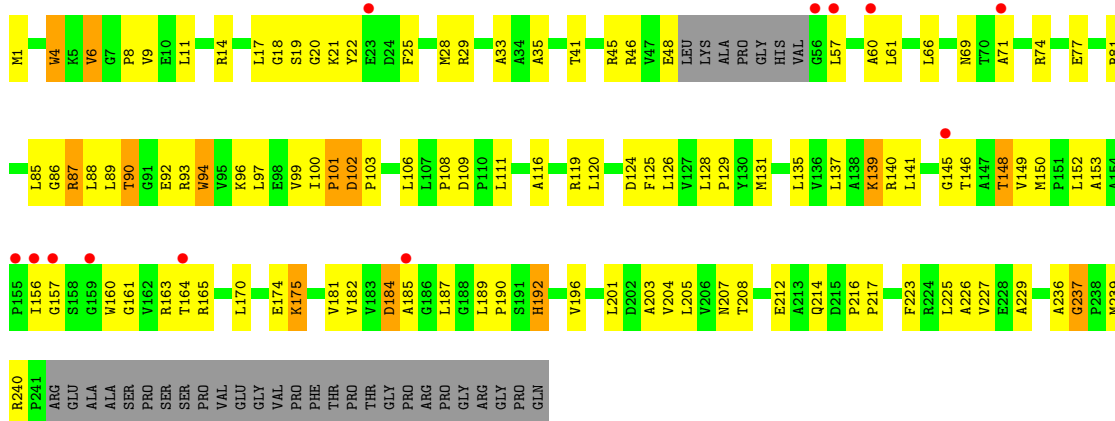


- Molecule 1: Thiazole biosynthesis protein thiG

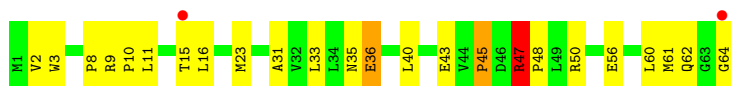




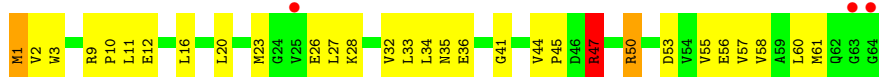
• Molecule 1: Thiazole biosynthesis protein thiG



• Molecule 2: Putative thiamine biosynthesis protein ThiS

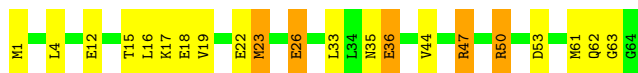


• Molecule 2: Putative thiamine biosynthesis protein ThiS



• Molecule 2: Putative thiamine biosynthesis protein ThiS





- Molecule 2: Putative thiamine biosynthesis protein ThiS



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	47.34Å 73.51Å 100.91Å 68.64° 80.16° 79.09°	Depositor
Resolution (Å)	19.96 – 2.30 19.96 – 2.31	Depositor EDS
% Data completeness (in resolution range)	97.7 (19.96-2.30) 97.6 (19.96-2.31)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.67 (at 2.30Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.253 , 0.266 0.252 , 0.265	Depositor DCC
R_{free} test set	2670 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	40.9	Xtrriage
Anisotropy	0.536	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 49.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9392	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.69% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.88	3/1789 (0.2%)	1.41	23/2433 (0.9%)
1	B	0.88	3/1780 (0.2%)	1.41	24/2421 (1.0%)
1	C	0.73	2/1842 (0.1%)	1.28	17/2507 (0.7%)
1	D	0.96	5/1789 (0.3%)	1.31	10/2433 (0.4%)
2	E	1.07	5/493 (1.0%)	1.47	5/662 (0.8%)
2	F	1.07	6/493 (1.2%)	1.51	5/662 (0.8%)
2	G	0.77	5/493 (1.0%)	1.18	2/662 (0.3%)
2	H	0.77	1/493 (0.2%)	1.19	2/662 (0.3%)
All	All	0.88	30/9172 (0.3%)	1.35	88/12442 (0.7%)

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	94	TRP	NE1-CE2	10.66	1.49	1.37
1	A	94	TRP	NE1-CE2	10.58	1.49	1.37
1	A	4	TRP	NE1-CE2	10.43	1.49	1.37
1	B	160	TRP	NE1-CE2	10.43	1.49	1.37
1	B	4	TRP	NE1-CE2	10.43	1.49	1.37
2	F	3	TRP	NE1-CE2	10.42	1.49	1.37
1	A	160	TRP	NE1-CE2	10.41	1.49	1.37
1	B	94	TRP	NE1-CE2	10.40	1.48	1.37
1	D	160	TRP	NE1-CE2	10.40	1.48	1.37
1	D	4	TRP	NE1-CE2	10.38	1.48	1.37
1	C	4	TRP	NE1-CE2	10.38	1.48	1.37
1	C	160	TRP	NE1-CE2	10.37	1.48	1.37
2	E	3	TRP	NE1-CE2	10.29	1.48	1.37
1	D	192	HIS	CG-CD2	5.77	1.42	1.35
2	G	1	MSE	SE-CE	-5.20	1.79	1.95
2	H	61	MSE	CG-SE	-5.17	1.79	1.95
2	F	61	MSE	CG-SE	-5.11	1.80	1.95
1	D	102	ASP	C-O	-5.11	1.20	1.25
2	G	61	MSE	CG-SE	-5.09	1.80	1.95
2	E	23	MSE	CG-SE	-5.08	1.80	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	23	MSE	CG-SE	-5.08	1.80	1.95
2	F	1	MSE	CG-SE	-5.07	1.80	1.95
2	E	61	MSE	CG-SE	-5.07	1.80	1.95
2	G	61	MSE	SE-CE	-5.04	1.80	1.95
2	E	23	MSE	SE-CE	-5.04	1.80	1.95
2	G	23	MSE	CG-SE	-5.03	1.80	1.95
2	G	23	MSE	SE-CE	-5.03	1.80	1.95
2	F	23	MSE	SE-CE	-5.02	1.80	1.95
2	E	61	MSE	SE-CE	-5.02	1.80	1.95
2	F	1	MSE	SE-CE	-5.01	1.80	1.95

All (88) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	101	PRO	N-CD-CG	7.21	114.02	103.20
1	B	102	ASP	CA-C-N	7.20	126.88	119.82
1	B	102	ASP	C-N-CA	7.20	126.88	119.82
1	A	129	PRO	N-CA-CB	7.00	106.84	102.92
1	C	129	PRO	N-CA-C	6.28	120.50	110.21
1	A	156	ILE	N-CA-C	6.13	117.33	109.30
1	B	149	VAL	CA-C-N	-6.10	115.66	123.16
1	B	149	VAL	C-N-CA	-6.10	115.66	123.16
2	H	47	ARG	CD-NE-CZ	-6.01	115.98	124.40
1	C	130	TYR	N-CA-C	-5.87	101.60	110.28
1	D	165	ARG	CD-NE-CZ	-5.67	116.46	124.40
2	F	10	PRO	N-CA-CB	5.61	106.49	102.28
1	A	238	PRO	N-CA-CB	5.56	108.19	103.35
2	E	10	PRO	N-CA-CB	5.46	106.07	102.25
1	C	165	ARG	CD-NE-CZ	-5.46	116.76	124.40
1	B	68	PRO	N-CA-CB	5.43	108.38	103.33
2	F	45	PRO	N-CA-CB	5.33	108.40	103.39
2	E	47	ARG	CD-NE-CZ	-5.28	117.00	124.40
2	E	45	PRO	N-CA-CB	5.28	108.01	103.31
1	A	173	ARG	CD-NE-CZ	-5.26	117.04	124.40
1	C	46	ARG	CD-NE-CZ	-5.20	117.12	124.40
1	B	163	ARG	CD-NE-CZ	-5.19	117.14	124.40
1	A	182	VAL	CA-C-N	-5.16	116.29	122.90
1	A	182	VAL	C-N-CA	-5.16	116.29	122.90
1	A	179	PRO	N-CA-CB	5.15	108.07	103.08
1	B	93	ARG	CD-NE-CZ	-5.14	117.20	124.40
1	B	46	ARG	CD-NE-CZ	-5.13	117.21	124.40
1	D	45	ARG	CD-NE-CZ	-5.13	117.22	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	8	PRO	N-CA-CB	5.13	107.40	103.30
1	A	65	ARG	CD-NE-CZ	-5.12	117.23	124.40
1	C	163	ARG	CD-NE-CZ	-5.12	117.23	124.40
2	F	9	ARG	CD-NE-CZ	-5.12	117.23	124.40
1	D	74	ARG	CD-NE-CZ	-5.11	117.24	124.40
1	A	240	ARG	CD-NE-CZ	-5.11	117.25	124.40
1	B	29	ARG	CD-NE-CZ	-5.11	117.25	124.40
1	B	173	ARG	CD-NE-CZ	-5.11	117.25	124.40
2	F	50	ARG	CD-NE-CZ	-5.10	117.26	124.40
1	C	93	ARG	CD-NE-CZ	-5.10	117.27	124.40
1	A	163	ARG	CD-NE-CZ	-5.10	117.27	124.40
1	A	126	LEU	CA-C-N	-5.09	115.80	122.37
1	A	126	LEU	C-N-CA	-5.09	115.80	122.37
1	A	119	ARG	CD-NE-CZ	-5.09	117.28	124.40
1	B	224	ARG	CD-NE-CZ	-5.09	117.28	124.40
2	G	47	ARG	CD-NE-CZ	-5.09	117.28	124.40
1	B	81	ARG	CD-NE-CZ	-5.09	117.28	124.40
1	C	84	ARG	CD-NE-CZ	-5.09	117.28	124.40
2	E	9	ARG	CD-NE-CZ	-5.08	117.28	124.40
2	G	50	ARG	CD-NE-CZ	-5.08	117.29	124.40
1	A	224	ARG	CD-NE-CZ	-5.08	117.29	124.40
1	B	84	ARG	CD-NE-CZ	-5.08	117.29	124.40
1	B	132	GLY	O-C-N	-5.08	116.24	122.03
1	A	84	ARG	CD-NE-CZ	-5.08	117.29	124.40
1	B	87	ARG	CD-NE-CZ	-5.08	117.29	124.40
1	B	231	ARG	CD-NE-CZ	-5.07	117.30	124.40
1	A	74	ARG	CD-NE-CZ	-5.07	117.30	124.40
1	B	119	ARG	CD-NE-CZ	-5.07	117.30	124.40
1	B	165	ARG	CD-NE-CZ	-5.07	117.30	124.40
1	C	87	ARG	CD-NE-CZ	-5.07	117.30	124.40
1	D	87	ARG	CD-NE-CZ	-5.07	117.30	124.40
1	D	163	ARG	CD-NE-CZ	-5.07	117.30	124.40
1	A	140	ARG	CD-NE-CZ	-5.07	117.31	124.40
1	C	45	ARG	CD-NE-CZ	-5.07	117.31	124.40
1	C	240	ARG	CD-NE-CZ	-5.07	117.31	124.40
1	A	81	ARG	CD-NE-CZ	-5.06	117.31	124.40
1	B	74	ARG	CD-NE-CZ	-5.06	117.31	124.40
1	A	68	PRO	N-CA-CB	5.06	107.56	103.36
1	A	93	ARG	CD-NE-CZ	-5.06	117.32	124.40
1	A	29	ARG	CD-NE-CZ	-5.06	117.32	124.40
2	H	9	ARG	CD-NE-CZ	-5.06	117.32	124.40
1	B	65	ARG	CD-NE-CZ	-5.05	117.34	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	240	ARG	CD-NE-CZ	-5.04	117.34	124.40
1	C	81	ARG	CD-NE-CZ	-5.04	117.34	124.40
1	D	81	ARG	CD-NE-CZ	-5.04	117.34	124.40
1	C	74	ARG	CD-NE-CZ	-5.04	117.34	124.40
1	B	103	PRO	N-CA-CB	5.04	108.31	103.52
1	C	65	ARG	CD-NE-CZ	-5.04	117.35	124.40
1	C	92	GLU	N-CA-C	5.04	118.33	110.32
1	D	140	ARG	CD-NE-CZ	-5.04	117.35	124.40
1	A	87	ARG	CD-NE-CZ	-5.03	117.35	124.40
1	A	165	ARG	CD-NE-CZ	-5.03	117.35	124.40
1	C	140	ARG	CD-NE-CZ	-5.03	117.36	124.40
1	D	240	ARG	CD-NE-CZ	-5.03	117.36	124.40
1	D	46	ARG	CD-NE-CZ	-5.03	117.36	124.40
1	B	45	ARG	CD-NE-CZ	-5.02	117.37	124.40
1	C	29	ARG	CD-NE-CZ	-5.02	117.38	124.40
1	C	14	ARG	CD-NE-CZ	-5.01	117.38	124.40
1	B	140	ARG	CD-NE-CZ	-5.01	117.39	124.40
2	F	47	ARG	CD-NE-CZ	-5.01	117.39	124.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [\(i\)](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1759	0	1844	107	0
1	B	1750	0	1838	86	0
1	C	1809	0	1900	115	0
1	D	1759	0	1844	101	0
2	E	489	0	503	21	0
2	F	489	0	503	17	0
2	G	489	0	503	20	0
2	H	489	0	503	20	0
3	A	89	0	0	5	0
3	B	60	0	0	0	0
3	C	94	0	0	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	58	0	0	5	0
3	E	10	0	0	0	0
3	F	14	0	0	0	0
3	G	30	0	0	1	0
3	H	4	0	0	1	0
All	All	9392	0	9438	441	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 24.

All (441) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:28:MET:HE3	1:C:61:LEU:HD21	1.16	1.14
1:B:40:VAL:HG23	1:B:64:VAL:HG11	1.38	1.06
1:A:45:ARG:HH11	1:A:45:ARG:HG2	1.30	0.95
1:A:156:ILE:HG12	1:A:185:ALA:HB1	1.51	0.92
2:F:36:GLU:HA	2:F:36:GLU:OE1	1.69	0.90
1:A:196:VAL:HG13	1:A:201:LEU:HD12	1.55	0.87
1:B:111:LEU:O	1:B:111:LEU:HD23	1.76	0.85
1:D:100:ILE:HG21	1:D:106:LEU:HA	1.58	0.84
1:A:120:LEU:O	1:A:125:PHE:HB2	1.77	0.83
1:C:28:MET:HE1	1:C:57:LEU:CD1	2.08	0.82
1:C:28:MET:CE	1:C:61:LEU:HD21	2.07	0.82
1:A:88:LEU:HD13	2:E:40:LEU:HD23	1.61	0.82
1:D:18:GLY:HA2	1:D:41:THR:HG22	1.61	0.82
1:A:111:LEU:HD13	1:D:111:LEU:HD13	1.62	0.82
1:B:40:VAL:CG2	1:B:64:VAL:HG11	2.10	0.81
2:H:9:ARG:HB3	2:H:11:LEU:HG	1.63	0.80
1:D:88:LEU:HD12	1:D:89:LEU:N	1.97	0.79
1:C:164:THR:HG22	1:C:164:THR:O	1.81	0.79
1:A:164:THR:HG22	1:A:164:THR:O	1.83	0.78
1:C:54:HIS:CE1	1:C:55:VAL:HG23	2.19	0.78
1:B:152:LEU:HA	1:B:184:ASP:O	1.84	0.78
1:B:106:LEU:HB3	1:B:156:ILE:HD12	1.66	0.77
1:B:184:ASP:HB2	1:B:205:LEU:HB3	1.65	0.76
1:D:196:VAL:HG13	1:D:201:LEU:HD12	1.66	0.76
1:A:4:TRP:H	1:A:4:TRP:CD1	2.01	0.76
1:A:239:MET:CE	1:B:159:GLY:HA3	2.15	0.76
1:C:133:PRO:HB3	1:C:164:THR:HG21	1.67	0.76
1:C:187:LEU:HD22	1:C:192:HIS:HB3	1.65	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:90:THR:CG2	1:D:92:GLU:H	2.00	0.75
1:B:120:LEU:O	1:B:125:PHE:HB2	1.86	0.75
1:C:94:TRP:HA	1:C:126:LEU:HB2	1.69	0.74
1:C:40:VAL:HG23	1:C:64:VAL:HG11	1.70	0.74
1:C:69:ASN:C	1:C:69:ASN:HD22	1.96	0.73
1:C:120:LEU:O	1:C:125:PHE:HB2	1.88	0.73
1:A:148:THR:HG22	1:A:149:VAL:N	2.02	0.73
1:C:164:THR:HG22	1:C:168:LEU:HG	1.69	0.73
1:C:28:MET:HE1	1:C:57:LEU:HD12	1.70	0.72
1:A:156:ILE:HG12	1:A:185:ALA:CB	2.19	0.71
1:C:38:GLU:O	1:C:64:VAL:HG13	1.89	0.71
1:C:85:LEU:HD11	2:G:33:LEU:HD11	1.73	0.71
1:B:41:THR:HA	1:B:67:LEU:O	1.89	0.71
1:A:41:THR:HG22	1:A:67:LEU:HB3	1.73	0.71
1:C:140:ARG:NH1	3:C:356:HOH:O	2.24	0.71
1:A:109:ASP:HB3	1:A:112:GLU:HB2	1.73	0.70
1:A:184:ASP:HB3	1:A:205:LEU:HB3	1.74	0.70
1:C:49:LEU:HG	2:G:23:MSE:HE3	1.74	0.69
1:A:239:MET:HE1	1:B:159:GLY:HA3	1.73	0.69
1:D:184:ASP:HB2	1:D:205:LEU:HB3	1.75	0.68
1:C:156:ILE:HG12	1:C:185:ALA:HB1	1.76	0.68
1:B:38:GLU:O	1:B:64:VAL:HG13	1.93	0.68
1:B:111:LEU:HD12	1:C:114:LEU:HD23	1.74	0.68
1:D:131:MET:HE3	1:D:137:LEU:HD23	1.75	0.68
1:D:150:MET:HG2	1:D:182:VAL:HB	1.75	0.68
1:D:28:MET:HE1	1:D:57:LEU:HD12	1.76	0.68
2:F:35:ASN:O	2:F:36:GLU:HB2	1.93	0.67
1:B:94:TRP:HD1	1:B:94:TRP:O	1.76	0.67
1:D:156:ILE:HG12	1:D:185:ALA:HB1	1.77	0.67
1:A:99:VAL:HG11	1:A:112:GLU:HB3	1.75	0.67
1:D:90:THR:HG23	1:D:92:GLU:H	1.60	0.67
1:C:196:VAL:HG13	1:C:201:LEU:HD12	1.77	0.66
1:D:88:LEU:HD12	1:D:88:LEU:C	2.21	0.66
1:D:187:LEU:CD1	1:D:204:VAL:HG13	2.25	0.66
1:C:133:PRO:HB3	1:C:164:THR:CG2	2.25	0.66
2:H:33:LEU:HB3	2:H:56:GLU:HB2	1.78	0.66
1:C:20:GLY:O	1:C:21:LYS:HB2	1.95	0.65
1:B:131:MET:HE3	1:B:137:LEU:HD23	1.77	0.65
1:B:69:ASN:HD22	1:B:69:ASN:C	2.03	0.65
1:A:4:TRP:H	1:A:4:TRP:HD1	1.45	0.65
1:C:6:VAL:HG13	1:C:9:VAL:HB	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:103:PRO:HA	1:D:106:LEU:HD23	1.79	0.65
1:B:41:THR:HG22	1:B:67:LEU:HD23	1.79	0.64
1:D:187:LEU:HD12	1:D:204:VAL:HG13	1.80	0.64
1:C:152:LEU:HA	1:C:184:ASP:O	1.96	0.64
1:C:182:VAL:HG22	1:C:203:ALA:HB3	1.78	0.64
1:A:223:PHE:O	1:A:227:VAL:HG23	1.99	0.63
2:G:26:GLU:HG2	3:G:68:HOH:O	1.97	0.63
1:A:184:ASP:OD1	1:A:184:ASP:N	2.31	0.63
1:B:187:LEU:HD22	1:B:192:HIS:HB3	1.80	0.63
1:D:128:LEU:HB3	1:D:148:THR:HG21	1.81	0.63
1:C:156:ILE:HG12	1:C:185:ALA:CB	2.29	0.62
1:C:225:LEU:HD22	1:D:225:LEU:HD22	1.80	0.62
1:A:103:PRO:HA	1:A:106:LEU:HD23	1.81	0.62
1:C:28:MET:HE3	1:C:61:LEU:CD2	2.10	0.62
1:A:128:LEU:HB3	1:A:150:MET:HE2	1.82	0.62
1:A:4:TRP:CD1	1:A:4:TRP:N	2.67	0.62
1:B:158:SER:HB2	1:B:160:TRP:CD1	2.34	0.62
1:C:148:THR:HG23	1:C:180:PRO:O	1.99	0.61
1:C:43:SER:CB	2:G:63:GLY:HA3	2.30	0.61
1:C:103:PRO:HA	1:C:106:LEU:HD23	1.81	0.61
1:B:28:MET:HE1	1:B:57:LEU:HD12	1.81	0.61
1:C:148:THR:HG22	1:C:149:VAL:N	2.14	0.61
1:A:105:TYR:O	1:A:106:LEU:HB2	1.99	0.61
1:C:54:HIS:NE2	1:C:55:VAL:HG23	2.15	0.61
1:D:41:THR:CG2	2:H:64:GLY:HA2	2.31	0.60
1:D:141:LEU:O	1:D:146:THR:HG23	2.01	0.60
1:C:49:LEU:HD23	1:C:49:LEU:C	2.26	0.60
1:B:184:ASP:O	1:B:185:ALA:HB3	2.01	0.60
1:C:164:THR:O	1:C:164:THR:CG2	2.48	0.60
1:D:29:ARG:HG3	1:D:60:ALA:HB1	1.82	0.60
1:D:61:LEU:HD13	1:D:66:LEU:HD22	1.84	0.60
1:A:58:LEU:HD21	2:E:60:LEU:HD12	1.83	0.60
1:C:94:TRP:CA	1:C:126:LEU:HB2	2.30	0.60
1:A:152:LEU:HA	1:A:184:ASP:O	2.02	0.59
1:B:14:ARG:NH1	1:B:14:ARG:HG2	2.17	0.59
1:C:135:LEU:HD22	1:C:170:LEU:HB3	1.83	0.59
1:B:205:LEU:C	1:B:205:LEU:HD23	2.28	0.59
1:B:87:ARG:NH2	1:B:123:GLU:O	2.36	0.59
1:B:100:ILE:HG21	1:B:106:LEU:HA	1.84	0.59
1:B:175:LYS:NZ	1:B:200:GLY:O	2.28	0.59
1:C:78:GLU:O	1:C:81:ARG:HB3	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:25:PHE:HB3	1:C:60:ALA:CB	2.33	0.59
2:E:40:LEU:HD12	2:E:43:GLU:OE1	2.03	0.59
1:A:197:MET:HE3	1:A:204:VAL:HG13	1.85	0.58
1:A:20:GLY:O	1:A:21:LYS:HB2	2.02	0.58
1:C:207:ASN:C	1:C:207:ASN:HD22	2.10	0.58
1:D:85:LEU:HD13	2:H:58:VAL:HG21	1.84	0.58
2:H:62:GLN:HG2	3:H:66:HOH:O	2.03	0.58
2:E:16:LEU:HD12	2:E:45:PRO:HD2	1.85	0.58
2:E:47:ARG:O	2:E:47:ARG:HG3	1.99	0.58
1:C:236:ALA:O	1:D:214:GLN:HB2	2.03	0.58
1:A:45:ARG:HG2	1:A:45:ARG:NH1	2.06	0.57
1:B:94:TRP:HA	1:B:126:LEU:HB2	1.85	0.57
1:C:25:PHE:HB3	1:C:60:ALA:HB2	1.87	0.57
1:A:69:ASN:C	1:A:69:ASN:HD22	2.10	0.57
1:B:148:THR:HA	1:B:179:PRO:HB2	1.86	0.57
1:C:225:LEU:HD22	1:D:225:LEU:CD2	2.33	0.57
1:A:23:GLU:O	1:A:24:ASP:HB3	2.05	0.57
1:D:77:GLU:HG3	3:D:275:HOH:O	2.02	0.57
1:D:128:LEU:HA	1:D:148:THR:HG22	1.84	0.57
2:H:47:ARG:HD3	2:H:48:PRO:O	2.03	0.57
1:D:120:LEU:O	1:D:125:PHE:HB2	2.04	0.57
1:A:142:ALA:HA	1:A:146:THR:HG22	1.87	0.57
1:A:94:TRP:HD1	1:A:94:TRP:O	1.88	0.57
1:A:148:THR:CG2	1:A:149:VAL:N	2.67	0.57
1:C:43:SER:HB2	2:G:63:GLY:HA3	1.85	0.57
1:B:197:MET:SD	1:B:227:VAL:HG13	2.45	0.56
1:D:184:ASP:CB	1:D:205:LEU:HB3	2.35	0.56
1:D:90:THR:HG22	1:D:92:GLU:H	1.70	0.56
2:E:2:VAL:HB	2:E:11:LEU:HB2	1.88	0.56
1:B:14:ARG:HG2	1:B:14:ARG:HH11	1.69	0.56
1:D:19:SER:O	1:D:22:TYR:HD2	1.88	0.56
1:A:19:SER:O	2:E:62:GLN:NE2	2.39	0.56
1:B:85:LEU:HD13	2:F:58:VAL:HG21	1.87	0.56
1:C:87:ARG:HD3	3:C:309:HOH:O	2.05	0.56
2:F:33:LEU:HB3	2:F:56:GLU:HB2	1.86	0.56
1:B:94:TRP:CD1	1:B:94:TRP:C	2.83	0.56
1:B:94:TRP:O	1:B:94:TRP:CD1	2.58	0.56
1:D:119:ARG:HG3	1:D:119:ARG:HH11	1.70	0.56
2:F:47:ARG:O	2:F:47:ARG:HG2	1.99	0.56
1:A:90:THR:HG22	2:E:60:LEU:HD11	1.88	0.56
1:D:4:TRP:H	1:D:4:TRP:CD1	2.24	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4:TRP:CD1	1:B:4:TRP:H	2.23	0.55
1:C:188:GLY:HA2	1:C:209:ALA:HB2	1.86	0.55
1:D:100:ILE:CG2	1:D:106:LEU:HA	2.35	0.55
1:A:133:PRO:HG3	1:A:164:THR:HG21	1.89	0.55
1:B:19:SER:O	1:B:22:TYR:HD2	1.89	0.55
1:B:128:LEU:HG	1:B:148:THR:HG22	1.88	0.55
1:B:111:LEU:HD23	1:B:111:LEU:C	2.31	0.55
1:C:16:ILE:O	1:C:17:LEU:HD23	2.06	0.55
1:A:65:ARG:NH2	3:A:297:HOH:O	2.27	0.55
1:A:101:PRO:O	1:A:103:PRO:HD3	2.06	0.55
1:C:184:ASP:HB2	1:C:205:LEU:HB3	1.89	0.55
1:C:100:ILE:HG21	1:C:106:LEU:HA	1.87	0.55
1:A:239:MET:HE2	1:B:159:GLY:HA3	1.87	0.55
1:A:41:THR:HG22	1:A:67:LEU:HD23	1.89	0.54
1:A:134:ASP:HB3	1:A:137:LEU:HB3	1.88	0.54
1:A:100:ILE:HG21	1:A:106:LEU:HA	1.90	0.54
1:D:152:LEU:HD12	1:D:152:LEU:O	2.07	0.54
1:A:189:LEU:O	1:A:192:HIS:HB2	2.07	0.54
1:C:6:VAL:HG22	1:C:6:VAL:O	2.06	0.54
1:D:129:PRO:HD2	1:D:148:THR:O	2.06	0.54
1:A:6:VAL:HG12	1:A:6:VAL:O	2.08	0.54
1:A:214:GLN:HG3	1:B:237:GLY:HA3	1.90	0.54
1:B:216:PRO:HB2	1:B:217:PRO:HD3	1.89	0.54
1:D:119:ARG:HG3	1:D:119:ARG:NH1	2.23	0.54
1:A:149:VAL:HG13	1:A:179:PRO:HG2	1.88	0.54
1:C:129:PRO:HD2	1:C:148:THR:O	2.08	0.54
1:C:214:GLN:HG3	1:D:237:GLY:HA3	1.90	0.53
2:E:33:LEU:HB3	2:E:56:GLU:HB2	1.89	0.53
1:B:58:LEU:HD21	2:F:60:LEU:HD12	1.89	0.53
1:C:19:SER:O	2:G:62:GLN:HB2	2.08	0.53
2:G:62:GLN:O	2:G:62:GLN:HG3	2.08	0.53
1:B:20:GLY:O	1:B:21:LYS:HB2	2.07	0.53
1:C:43:SER:HA	1:C:69:ASN:ND2	2.23	0.53
1:C:184:ASP:O	1:C:185:ALA:HB3	2.09	0.53
1:B:35:ALA:O	1:B:36:LYS:HB2	2.08	0.53
1:A:165:ARG:HG2	1:A:165:ARG:HH11	1.72	0.53
1:B:4:TRP:CD1	1:B:4:TRP:N	2.77	0.53
1:B:153:ALA:HB3	1:B:186:GLY:HA3	1.90	0.52
1:A:17:LEU:CD2	1:A:210:ILE:HD12	2.39	0.52
1:D:128:LEU:HB3	1:D:148:THR:CG2	2.39	0.52
1:B:208:THR:HG23	1:B:212:GLU:HG3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:61:LEU:HB3	1:D:66:LEU:HD21	1.91	0.52
1:A:121:ILE:HG13	1:A:127:VAL:HG23	1.91	0.52
1:A:164:THR:O	1:A:164:THR:CG2	2.54	0.52
1:C:92:GLU:HG2	3:C:274:HOH:O	2.08	0.52
1:C:35:ALA:O	1:C:224:ARG:HG3	2.10	0.52
2:G:4:LEU:HD21	2:G:23:MSE:SE	2.60	0.52
1:C:159:GLY:HA3	1:D:239:MET:HE2	1.91	0.52
1:D:88:LEU:C	1:D:88:LEU:CD1	2.83	0.52
2:E:15:THR:HG22	2:E:16:LEU:N	2.25	0.52
1:A:41:THR:HA	1:A:67:LEU:O	2.09	0.51
1:C:59:GLU:O	1:C:59:GLU:HG2	2.09	0.51
1:A:133:PRO:HB3	1:A:164:THR:HG21	1.93	0.51
1:D:8:PRO:HD2	1:D:126:LEU:HD11	1.93	0.51
1:A:123:GLU:O	1:A:124:ASP:HB3	2.11	0.51
1:A:165:ARG:HG2	1:A:165:ARG:NH1	2.26	0.51
1:D:184:ASP:O	1:D:185:ALA:HB3	2.11	0.51
2:F:26:GLU:N	2:F:26:GLU:OE1	2.43	0.51
2:G:12:GLU:HG3	2:G:50:ARG:HA	1.92	0.51
1:A:133:PRO:HG3	1:A:164:THR:CG2	2.41	0.50
1:C:43:SER:HA	1:C:69:ASN:HD21	1.77	0.50
1:B:148:THR:HG23	1:B:149:VAL:N	2.25	0.50
1:D:187:LEU:HD12	1:D:204:VAL:CG1	2.41	0.50
1:C:119:ARG:O	1:C:122:GLU:HG2	2.12	0.50
1:D:96:LYS:HG3	1:D:150:MET:HE1	1.93	0.50
2:F:1:MSE:N	2:F:12:GLU:OE1	2.43	0.50
1:D:223:PHE:O	1:D:227:VAL:HG23	2.11	0.50
2:F:2:VAL:HB	2:F:11:LEU:HB2	1.93	0.50
1:B:107:LEU:HD11	1:C:170:LEU:HD12	1.94	0.50
1:C:134:ASP:HB3	1:C:137:LEU:HB3	1.94	0.50
1:D:139:LYS:NZ	1:D:174:GLU:OE1	2.39	0.50
1:D:148:THR:CG2	1:D:150:MET:HG3	2.42	0.50
1:A:150:MET:HA	1:A:182:VAL:O	2.12	0.49
1:B:99:VAL:HG11	1:B:112:GLU:HB3	1.93	0.49
1:C:131:MET:HE1	1:C:138:ALA:HA	1.94	0.49
1:D:20:GLY:HA2	2:H:62:GLN:HB2	1.93	0.49
1:C:43:SER:OG	2:G:63:GLY:HA3	2.12	0.49
1:A:73:ALA:HB2	1:A:82:LEU:HD12	1.94	0.49
1:C:28:MET:HE1	1:C:57:LEU:HD11	1.91	0.49
1:C:69:ASN:C	1:C:69:ASN:ND2	2.67	0.49
1:C:184:ASP:CB	1:C:205:LEU:HB3	2.42	0.49
1:D:148:THR:HG23	1:D:150:MET:HG3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:148:THR:CG2	1:C:149:VAL:N	2.75	0.49
1:C:164:THR:CG2	1:C:168:LEU:HG	2.39	0.49
2:H:11:LEU:O	2:H:14:LYS:HB2	2.13	0.49
1:C:28:MET:CE	1:C:57:LEU:HD12	2.42	0.49
1:C:94:TRP:CB	1:C:126:LEU:HB2	2.43	0.49
1:D:25:PHE:CD1	1:D:25:PHE:N	2.80	0.49
1:C:216:PRO:HB2	1:C:217:PRO:HD3	1.95	0.48
1:D:41:THR:HG23	2:H:64:GLY:HA2	1.94	0.48
2:G:47:ARG:NH2	2:G:53:ASP:OD2	2.46	0.48
1:A:94:TRP:CD1	1:A:94:TRP:C	2.91	0.48
1:D:101:PRO:HG3	1:D:109:ASP:HB2	1.94	0.48
1:A:90:THR:HG22	2:E:60:LEU:CD1	2.43	0.48
1:C:156:ILE:CG1	1:C:185:ALA:HB1	2.41	0.48
1:D:4:TRP:CD1	1:D:4:TRP:N	2.81	0.48
1:A:102:ASP:HB3	3:A:355:HOH:O	2.13	0.48
1:A:148:THR:HG22	1:A:149:VAL:H	1.75	0.48
1:B:65:ARG:HD3	1:B:92:GLU:OE2	2.13	0.48
1:C:99:VAL:HG11	1:C:112:GLU:HB3	1.95	0.48
1:A:41:THR:HG22	1:A:67:LEU:CB	2.42	0.48
1:D:85:LEU:O	1:D:89:LEU:HB2	2.12	0.48
1:A:57:LEU:HG	1:A:61:LEU:HD12	1.95	0.48
1:B:105:TYR:O	1:B:106:LEU:HB2	2.12	0.48
1:A:88:LEU:HD12	1:A:88:LEU:C	2.38	0.48
2:E:35:ASN:O	2:E:36:GLU:HB2	2.13	0.48
1:A:43:SER:HA	1:A:69:ASN:ND2	2.28	0.48
1:A:160:TRP:HB3	1:A:163:ARG:HE	1.79	0.48
1:D:94:TRP:HD1	1:D:94:TRP:O	1.96	0.48
2:F:27:LEU:O	2:F:41:GLY:HA3	2.12	0.48
1:C:78:GLU:HB3	3:C:314:HOH:O	2.14	0.47
1:D:86:GLY:O	1:D:90:THR:HB	2.13	0.47
1:A:12:LYS:N	1:A:12:LYS:HD2	2.28	0.47
1:C:49:LEU:HD23	1:C:49:LEU:O	2.13	0.47
2:H:35:ASN:O	2:H:36:GLU:HB2	2.14	0.47
1:D:190:PRO:HB3	1:D:226:ALA:HB2	1.96	0.47
1:A:36:LYS:HG3	1:A:224:ARG:HD2	1.96	0.47
1:B:150:MET:HA	1:B:182:VAL:O	2.14	0.47
1:D:97:LEU:HD21	1:D:116:ALA:HB3	1.96	0.47
2:F:34:LEU:HD12	2:F:55:VAL:HG22	1.96	0.47
1:C:102:ASP:HB3	3:C:327:HOH:O	2.13	0.47
1:A:41:THR:OG1	2:E:64:GLY:HA3	2.14	0.47
1:C:54:HIS:NE2	1:C:55:VAL:CG2	2.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:94:TRP:HB3	1:C:126:LEU:HB2	1.97	0.47
1:C:233:ALA:HB2	1:D:190:PRO:HG2	1.96	0.47
1:D:41:THR:HG21	2:H:64:GLY:HA2	1.96	0.47
1:D:90:THR:CG2	1:D:92:GLU:HB2	2.44	0.47
2:H:35:ASN:C	2:H:36:GLU:HG3	2.39	0.47
1:A:151:PRO:HB2	1:A:168:LEU:HD21	1.97	0.47
1:A:69:ASN:C	1:A:69:ASN:ND2	2.73	0.47
1:A:225:LEU:HB2	1:B:229:ALA:HB2	1.96	0.47
1:C:135:LEU:O	1:C:138:ALA:HB3	2.15	0.47
1:C:239:MET:O	1:C:239:MET:HG3	2.13	0.47
1:C:176:ALA:HA	3:C:312:HOH:O	2.15	0.46
1:D:102:ASP:HA	1:D:103:PRO:HD3	1.74	0.46
2:F:36:GLU:OE1	2:F:36:GLU:CA	2.44	0.46
1:D:216:PRO:HB2	1:D:217:PRO:HD3	1.97	0.46
2:G:50:ARG:HG2	2:G:53:ASP:OD2	2.14	0.46
1:A:74:ARG:HE	1:A:74:ARG:HB2	1.63	0.46
1:B:27:VAL:HG11	1:B:216:PRO:HG2	1.97	0.46
1:C:95:VAL:HG11	1:C:120:LEU:HD13	1.97	0.46
1:C:163:ARG:NH2	3:C:280:HOH:O	2.48	0.46
1:A:239:MET:HE1	1:B:159:GLY:CA	2.44	0.46
2:G:15:THR:O	2:G:19:VAL:HG23	2.15	0.46
1:B:96:LYS:HA	1:B:128:LEU:O	2.15	0.46
1:D:14:ARG:HG2	1:D:14:ARG:HH11	1.80	0.46
1:C:42:VAL:HG11	1:C:66:LEU:HD22	1.97	0.46
2:G:47:ARG:NH2	2:G:53:ASP:CG	2.74	0.46
2:H:47:ARG:HH12	2:H:53:ASP:CG	2.23	0.46
1:B:196:VAL:HG13	1:B:201:LEU:HD12	1.97	0.46
1:C:87:ARG:NH1	1:C:124:ASP:O	2.45	0.46
1:D:152:LEU:HD12	1:D:152:LEU:C	2.41	0.46
1:A:43:SER:HA	1:A:69:ASN:HD21	1.80	0.46
1:A:87:ARG:O	1:A:91:GLY:N	2.45	0.46
1:A:135:LEU:HD21	1:A:174:GLU:HG3	1.97	0.46
1:C:93:ARG:HH11	1:C:93:ARG:HD3	1.62	0.46
2:F:16:LEU:HD13	2:F:44:VAL:HB	1.98	0.46
1:A:85:LEU:HD21	2:E:33:LEU:HB2	1.98	0.45
1:B:148:THR:O	1:B:149:VAL:HG13	2.16	0.45
1:D:208:THR:CG2	1:D:212:GLU:HG3	2.46	0.45
1:B:40:VAL:HG23	1:B:64:VAL:CG1	2.27	0.45
1:D:128:LEU:HD22	1:D:148:THR:HB	1.99	0.45
1:D:153:ALA:O	1:D:164:THR:HG23	2.17	0.45
1:D:187:LEU:CD1	1:D:204:VAL:CG1	2.93	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:LEU:HG	2:E:31:ALA:HB2	1.97	0.45
1:C:49:LEU:C	1:C:49:LEU:CD2	2.90	0.45
1:C:207:ASN:C	1:C:207:ASN:ND2	2.75	0.45
1:B:221:GLU:O	1:B:224:ARG:HB3	2.16	0.45
1:C:240:ARG:HH11	1:C:240:ARG:HD3	1.64	0.45
1:A:59:GLU:HG2	3:A:333:HOH:O	2.16	0.45
1:B:47:VAL:HG13	2:F:57:VAL:O	2.17	0.45
1:B:152:LEU:H	1:B:152:LEU:HG	1.63	0.45
2:H:17:LYS:O	2:H:21:GLU:HB2	2.17	0.45
1:C:240:ARG:H	1:C:240:ARG:HG2	1.60	0.44
1:B:150:MET:HB3	1:B:182:VAL:O	2.17	0.44
1:C:190:PRO:HB3	1:C:226:ALA:HB2	1.98	0.44
1:C:193:ALA:HB2	1:C:223:PHE:HE1	1.81	0.44
1:C:225:LEU:CD2	1:D:225:LEU:HD22	2.47	0.44
1:B:128:LEU:HA	1:B:148:THR:HG22	1.99	0.44
1:A:45:ARG:NH1	1:A:45:ARG:CG	2.72	0.44
1:A:175:LYS:HB2	1:A:175:LYS:HE3	1.80	0.44
1:A:233:ALA:HB2	1:B:190:PRO:HG2	2.00	0.44
1:C:214:GLN:HB2	1:D:236:ALA:O	2.17	0.44
1:A:28:MET:HE1	1:A:57:LEU:CD1	2.47	0.44
1:B:108:PRO:HG2	1:B:131:MET:HA	1.99	0.44
1:C:43:SER:HB2	2:G:63:GLY:CA	2.48	0.44
1:C:208:THR:O	1:C:212:GLU:HB2	2.18	0.44
2:F:20:LEU:HD11	2:F:32:VAL:HG21	1.99	0.44
1:A:148:THR:CG2	1:A:149:VAL:H	2.31	0.44
1:A:154:ALA:HB1	1:A:155:PRO:HD2	1.98	0.44
1:C:96:LYS:NZ	3:C:272:HOH:O	2.50	0.44
1:D:106:LEU:HD12	1:D:156:ILE:HB	1.99	0.44
1:D:161:GLY:HA2	1:D:192:HIS:ND1	2.33	0.44
1:B:128:LEU:HG	1:B:148:THR:CG2	2.48	0.44
1:B:149:VAL:C	1:B:150:MET:HG2	2.42	0.44
2:F:12:GLU:O	2:F:12:GLU:HG2	2.17	0.44
1:A:88:LEU:HD12	1:A:89:LEU:N	2.33	0.43
1:B:168:LEU:HD23	1:B:168:LEU:HA	1.89	0.43
1:B:197:MET:HE3	1:B:197:MET:HA	2.00	0.43
1:D:17:LEU:HD11	1:D:35:ALA:HB3	2.00	0.43
1:D:33:ALA:HA	3:D:288:HOH:O	2.18	0.43
1:B:109:ASP:HB3	1:B:112:GLU:HB2	1.99	0.43
1:B:207:ASN:C	1:B:207:ASN:HD22	2.25	0.43
1:C:32:ILE:HG21	1:C:64:VAL:HG21	2.00	0.43
1:A:148:THR:HG23	1:A:180:PRO:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:5:LYS:O	3:C:290:HOH:O	2.21	0.43
1:D:69:ASN:OD1	1:D:71:ALA:CB	2.67	0.43
1:C:139:LYS:HG2	1:C:178:LEU:HD21	2.00	0.43
2:E:47:ARG:HA	2:E:48:PRO:HD3	1.88	0.43
2:G:18:GLU:O	2:G:22:GLU:HB2	2.19	0.43
2:H:47:ARG:HD2	2:H:47:ARG:O	2.19	0.43
1:C:35:ALA:O	1:C:36:LYS:HB2	2.17	0.43
2:H:15:THR:O	2:H:19:VAL:HG23	2.19	0.43
1:C:150:MET:HA	1:C:182:VAL:O	2.18	0.43
1:A:106:LEU:HD12	1:A:156:ILE:HB	2.00	0.43
2:E:47:ARG:HH11	2:E:47:ARG:HD2	1.59	0.43
2:H:35:ASN:O	2:H:36:GLU:CB	2.67	0.43
1:B:45:ARG:HG2	1:B:45:ARG:HH11	1.83	0.42
1:B:135:LEU:HD21	1:B:174:GLU:HG3	2.00	0.42
1:B:148:THR:OG1	1:B:180:PRO:O	2.32	0.42
1:A:94:TRP:O	1:A:94:TRP:CD1	2.69	0.42
1:A:88:LEU:HB2	2:E:40:LEU:HD21	2.01	0.42
1:A:123:GLU:O	1:A:124:ASP:CB	2.67	0.42
1:A:216:PRO:HB2	1:A:217:PRO:HD3	2.02	0.42
1:D:6:VAL:HG13	1:D:9:VAL:HB	2.02	0.42
1:C:142:ALA:HA	1:C:146:THR:HG22	2.00	0.42
1:D:208:THR:HG23	1:D:212:GLU:HG3	2.01	0.42
2:F:50:ARG:O	2:F:53:ASP:HB2	2.19	0.42
2:G:47:ARG:HH22	2:G:53:ASP:CG	2.27	0.42
1:A:41:THR:CG2	1:A:67:LEU:HD23	2.50	0.42
1:C:151:PRO:HB2	1:C:168:LEU:HD21	2.02	0.42
1:D:14:ARG:HG2	1:D:14:ARG:NH1	2.35	0.42
1:D:184:ASP:OD1	1:D:184:ASP:C	2.61	0.42
1:B:14:ARG:HH11	1:B:14:ARG:CG	2.31	0.42
1:D:181:VAL:HG11	1:D:201:LEU:HD22	2.02	0.42
2:H:47:ARG:NH1	2:H:53:ASP:OD2	2.50	0.42
1:A:5:LYS:HA	1:A:9:VAL:O	2.19	0.42
1:B:69:ASN:C	1:B:69:ASN:ND2	2.75	0.42
1:B:129:PRO:CG	1:B:141:LEU:HD13	2.50	0.42
1:C:92:GLU:CG	3:C:274:HOH:O	2.68	0.42
1:C:4:TRP:H	1:C:4:TRP:CD1	2.38	0.41
1:C:36:LYS:HB2	1:C:224:ARG:HD2	2.01	0.41
1:D:87:ARG:NH2	1:D:124:ASP:O	2.53	0.41
1:A:59:GLU:OE2	3:A:281:HOH:O	2.21	0.41
2:H:25:VAL:HG21	2:H:30:VAL:HG11	2.02	0.41
1:A:184:ASP:O	1:A:185:ALA:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:MET:HA	1:A:197:MET:HE2	2.00	0.41
1:D:207:ASN:C	1:D:207:ASN:ND2	2.77	0.41
1:A:25:PHE:N	1:A:25:PHE:CD1	2.87	0.41
1:A:156:ILE:HD13	3:A:277:HOH:O	2.20	0.41
1:B:81:ARG:HH11	1:B:81:ARG:HD2	1.63	0.41
1:B:94:TRP:CA	1:B:126:LEU:HB2	2.50	0.41
1:D:175:LYS:HB2	1:D:175:LYS:HE3	1.67	0.41
1:D:227:VAL:HB	3:D:293:HOH:O	2.21	0.41
1:B:108:PRO:HG3	1:B:130:TYR:CE2	2.56	0.41
1:D:4:TRP:CD1	1:D:11:LEU:O	2.74	0.41
1:D:145:GLY:O	3:D:309:HOH:O	2.22	0.41
1:A:152:LEU:H	1:A:152:LEU:HG	1.75	0.41
1:B:129:PRO:HG2	1:B:141:LEU:HD13	2.03	0.41
1:C:239:MET:HE1	1:D:157:GLY:O	2.19	0.41
1:D:20:GLY:C	1:D:21:LYS:HG2	2.45	0.41
1:D:135:LEU:HD22	1:D:170:LEU:HB3	2.00	0.41
1:D:189:LEU:HB2	1:D:192:HIS:CE1	2.56	0.41
2:E:35:ASN:O	2:E:36:GLU:CB	2.68	0.41
1:B:167:LEU:HD23	1:B:170:LEU:HD12	2.01	0.41
1:C:154:ALA:HB1	1:C:155:PRO:HD2	2.03	0.41
2:G:35:ASN:O	2:G:36:GLU:CB	2.69	0.41
1:D:128:LEU:CA	1:D:148:THR:HG22	2.51	0.41
1:D:182:VAL:HG22	1:D:203:ALA:HB3	2.03	0.41
2:E:50:ARG:HH11	2:E:50:ARG:HD2	1.64	0.41
2:G:35:ASN:O	2:G:36:GLU:HB2	2.21	0.41
1:B:189:LEU:O	1:B:192:HIS:HB2	2.21	0.41
1:C:225:LEU:HB2	1:D:229:ALA:HB2	2.02	0.41
1:D:89:LEU:HG	2:H:31:ALA:HB2	2.03	0.41
1:D:99:VAL:O	1:D:108:PRO:HA	2.21	0.41
2:G:16:LEU:HD12	2:G:44:VAL:HB	2.03	0.41
1:A:17:LEU:HD22	1:A:210:ILE:HD12	2.03	0.40
1:A:108:PRO:HG2	1:A:131:MET:HA	2.03	0.40
1:D:152:LEU:H	1:D:152:LEU:HG	1.67	0.40
1:A:208:THR:O	1:A:212:GLU:HB2	2.21	0.40
1:B:123:GLU:O	1:B:124:ASP:CB	2.69	0.40
1:C:119:ARG:NH1	3:C:354:HOH:O	2.54	0.40
1:A:90:THR:CG2	2:E:60:LEU:HD11	2.50	0.40
1:B:149:VAL:HG23	1:B:181:VAL:HG22	2.04	0.40
1:C:120:LEU:C	1:C:125:PHE:HB2	2.45	0.40
1:A:41:THR:HG22	1:A:67:LEU:CG	2.51	0.40
1:A:35:ALA:O	1:A:36:LYS:HB2	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:205:LEU:C	1:B:205:LEU:CD2	2.94	0.40
1:D:77:GLU:CG	3:D:275:HOH:O	2.67	0.40
1:D:152:LEU:HA	1:D:184:ASP:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	230/268 (86%)	217 (94%)	13 (6%)	0	100	100
1	B	229/268 (85%)	214 (93%)	14 (6%)	1 (0%)	30	38
1	C	239/268 (89%)	224 (94%)	15 (6%)	0	100	100
1	D	230/268 (86%)	213 (93%)	16 (7%)	1 (0%)	30	38
2	E	62/64 (97%)	60 (97%)	2 (3%)	0	100	100
2	F	62/64 (97%)	61 (98%)	1 (2%)	0	100	100
2	G	62/64 (97%)	57 (92%)	5 (8%)	0	100	100
2	H	62/64 (97%)	61 (98%)	1 (2%)	0	100	100
All	All	1176/1328 (89%)	1107 (94%)	67 (6%)	2 (0%)	43	55

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	237	GLY
1	D	237	GLY

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	179/205 (87%)	162 (90%)	17 (10%)	8	10
1	B	178/205 (87%)	160 (90%)	18 (10%)	7	9
1	C	184/205 (90%)	174 (95%)	10 (5%)	20	29
1	D	179/205 (87%)	169 (94%)	10 (6%)	19	28
2	E	53/50 (106%)	51 (96%)	2 (4%)	29	44
2	F	53/50 (106%)	51 (96%)	2 (4%)	29	44
2	G	53/50 (106%)	50 (94%)	3 (6%)	18	27
2	H	53/50 (106%)	51 (96%)	2 (4%)	29	44
All	All	932/1020 (91%)	868 (93%)	64 (7%)	14	20

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	19	SER
1	A	29	ARG
1	A	43	SER
1	A	48	GLU
1	A	58	LEU
1	A	59	GLU
1	A	69	ASN
1	A	74	ARG
1	A	77	GLU
1	A	115	LYS
1	A	119	ARG
1	A	120	LEU
1	A	122	GLU
1	A	175	LYS
1	A	239	MET
1	A	240	ARG
1	B	45	ARG
1	B	47	VAL

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Mol	Chain	Res	Type
1	B	65	ARG
1	B	69	ASN
1	B	77	GLU
1	B	92	GLU
1	B	115	LYS
1	B	119	ARG
1	B	120	LEU
1	B	121	ILE
1	B	140	ARG
1	B	150	MET
1	B	165	ARG
1	B	169	GLU
1	B	175	LYS
1	B	184	ASP
1	B	197	MET
1	B	224	ARG
1	C	5	LYS
1	C	6	VAL
1	C	45	ARG
1	C	48	GLU
1	C	62	GLU
1	C	69	ASN
1	C	74	ARG
1	C	92	GLU
1	C	146	THR
1	C	214	GLN
1	D	1	MET
1	D	6	VAL
1	D	48	GLU
1	D	90	THR
1	D	93	ARG
1	D	139	LYS
1	D	148	THR
1	D	149	VAL
1	D	175	LYS
1	D	184	ASP
2	E	36	GLU
2	E	47	ARG
2	F	28	LYS
2	F	47	ARG
2	G	17	LYS
2	G	26	GLU

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Mol	Chain	Res	Type
2	G	36	GLU
2	H	9	ARG
2	H	17	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	69	ASN
1	B	69	ASN
1	B	207	ASN
1	C	69	ASN
1	C	207	ASN
1	C	214	GLN
1	D	207	ASN
1	D	214	GLN
2	G	62	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	234/268 (87%)	0.40	9 (3%) 44 46	24, 40, 59, 74	0
1	B	233/268 (86%)	0.48	12 (5%) 33 34	20, 39, 60, 73	0
1	C	241/268 (89%)	0.46	8 (3%) 49 51	32, 45, 66, 83	0
1	D	234/268 (87%)	0.43	12 (5%) 33 35	33, 44, 66, 82	0
2	E	61/64 (95%)	0.67	2 (3%) 49 51	35, 56, 69, 76	0
2	F	61/64 (95%)	0.58	3 (4%) 35 36	36, 57, 69, 75	0
2	G	61/64 (95%)	0.34	0 100 100	39, 50, 67, 71	0
2	H	61/64 (95%)	0.80	4 (6%) 24 26	48, 68, 79, 90	0
All	All	1186/1328 (89%)	0.47	50 (4%) 40 42	20, 45, 69, 90	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	156	ILE	8.2
1	A	156	ILE	5.1
1	C	49	LEU	4.4
1	C	51	ALA	4.0
1	B	155	PRO	3.8
1	D	156	ILE	3.8
2	E	64	GLY	3.6
1	D	157	GLY	3.4
1	A	155	PRO	3.4
1	C	55	VAL	3.4
2	H	11	LEU	3.2
1	C	61	LEU	3.0
2	F	64	GLY	2.9
1	A	48	GLU	2.9
1	C	1	MET	2.7
1	B	157	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
2	H	63	GLY	2.7
1	D	155	PRO	2.6
1	A	106	LEU	2.6
1	D	56	GLY	2.5
2	E	15	THR	2.5
1	D	60	ALA	2.5
2	H	36	GLU	2.5
1	B	185	ALA	2.5
1	D	164	THR	2.4
1	D	57	LEU	2.4
1	B	160	TRP	2.4
2	H	64	GLY	2.3
1	C	6	VAL	2.3
2	F	25	VAL	2.3
1	B	77	GLU	2.3
1	C	156	ILE	2.3
1	B	64	VAL	2.3
2	F	63	GLY	2.2
1	A	122	GLU	2.2
1	D	145	GLY	2.2
1	B	154	ALA	2.2
1	D	159	GLY	2.1
1	D	185	ALA	2.1
1	A	1	MET	2.1
1	A	145	GLY	2.1
1	B	176	ALA	2.1
1	B	204	VAL	2.1
1	D	71	ALA	2.1
1	B	58	LEU	2.1
1	B	241	PRO	2.1
1	A	18	GLY	2.1
1	C	54	HIS	2.0
1	A	163	ARG	2.0
1	D	23	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [\(i\)](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.